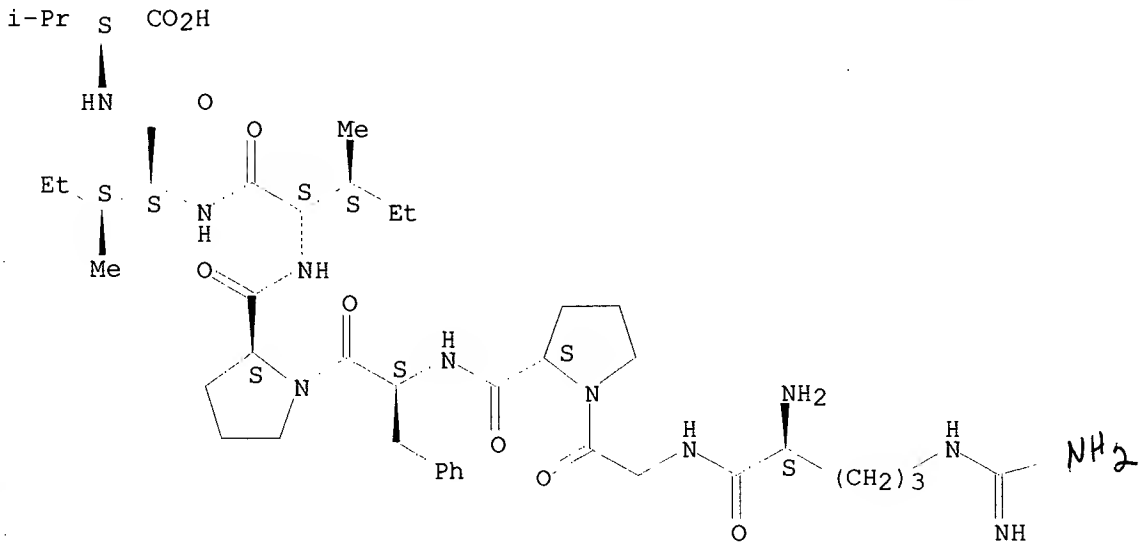
```
=> fil reg; d que l9
FILE 'REGISTRY' ENTERED AT 15:54:19 ON 27 FEB 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   26 FEB 2003  HIGHEST RN 495373-62-1
DICTIONARY FILE UPDATES:  26 FEB 2003  HIGHEST RN 495373-62-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available.  See HELP
PROPERTIES for more information.  See STNote 27, Searching Properties
in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf


L1          196 SEA FILE=REGISTRY ABB=ON  .BETA.(L)CASEIN#
L2           96 SEA FILE=REGISTRY ABB=ON  L1 AND PS/FS
L3         2853 SEA FILE=REGISTRY ABB=ON  BOVINE
L4            2 SEA FILE=REGISTRY ABB=ON  L2 AND L3
L8          661 SEA FILE=REGISTRY ABB=ON  PGPI[HP]/SQSP
L9            1 SEA FILE=REGISTRY ABB=ON  L4 NOT L8

=> d rn cn sql kwic nte lc l9

L9   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2003 ACS
RN   90600-53-6  REGISTRY
CN   L-Valine, N-[N-[N-[1-[N-[1-(N-L-arginylglycyl)-L-prolyl]-L-phenylalanyl]-L-
     prolyl]-L-isoleucyl]-L-isoleucyl]- (9CI)  (CA INDEX NAME)
OTHER NAMES:
CN   Bovine .beta.-casein (202-209)
SQL  8
OTHER NAMES:
CN   Bovine .beta.-casein (202-209)
FS   PROTEIN SEQUENCE; STEREOSEARCH
LC   STN Files:   CA, CAPLUS


=> d sqide

L9   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2003 ACS
RN   90600-53-6  REGISTRY
CN   L-Valine, N-[N-[N-[1-[N-[1-(N-L-arginylglycyl)-L-prolyl]-L-phenylalanyl]-L-
     prolyl]-L-isoleucyl]-L-isoleucyl]- (9CI)  (CA INDEX NAME)
OTHER NAMES:
CN   Bovine .beta.-casein (202-209)
FS   PROTEIN SEQUENCE; STEREOSEARCH
SQL  8

SEQ      1 RGPFPIIV

**RELATED SEQUENCES AVAILABLE WITH SEQLINK**
MF   C44 H71 N11 O9
```

CI COM
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

NH2

8 REFERENCES IN FILE CA (1962 TO DATE)
8 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> fil capl; s 19
FILE 'CAPLUS' ENTERED AT 15:55:28 ON 27 FEB 2003

FILE COVERS 1907 - 27 Feb 2003 VOL 138 ISS 9
FILE LAST UPDATED: 26 Feb 2003 (20030226/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

L10 8 L9

=> d ibib ab hitrn 1-8

L10 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:624529 CAPLUS
DOCUMENT NUMBER: 123:221057
TITLE: Conversion of bitterness of C-terminal octapeptide of bovine .beta.-casein (Arg-Gly-Pro-Phe-Pro-Ile-Ile-Val) into sweetness
AUTHOR(S): Takahashi, Masatoshi; Nakata, Takashi; Nakatani, Masaru; Kataoka, Shiro; Nakamura, Kozo; Okai, Hideo
CORPORATE SOURCE: Faculty Engineering, Hiroshima University, Higashi-Hiroshima, 724, Japan
SOURCE: Peptide Chemistry (1995), Volume Date 1994, 32nd, 281-4
CODEN: PECHDP; ISSN: 0388-3698
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The bitterness/sweetness taste of a series of peptides related to the title bitter .beta.-casein C-terminal octapeptide (I) was investigated. It was found that substituting Glu for Phe in I produced slight sweetness with bitterness and substituting Glu for Gly in I produced sweetness which was 1000-fold stronger than sucrose along with bitterness. A I analog in which both Arg and Phe were substituted by Glu residues produced sweetness which was 667-fold stronger than sucrose and no bitterness. The reasons for these changes in organoleptic properties were discussed and a model for sweet and bitter taste recognition by a single taste receptor was described.
IT **90600-53-6**
RL: PRP (Properties)
(bitterness/sweetness of bovine .beta.-casein C-terminal octapeptide analogs)

L10 ANSWER 2 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:457946 CAPLUS
DOCUMENT NUMBER: 121:57946
TITLE: Studies on bitter peptides from casein hydrolyzate. XIV. Bitter taste of synthetic analogs of octapeptide, Arg-Gly-Pro-Phe-Pro-Ile-Ile-Val, corresponding to the C-terminal portion of .beta.-casein
AUTHOR(S): Nakatani, Masaru; Nakata, Takashi; Kouge, Katsushige; Okai, Hideo
CORPORATE SOURCE: Fac. Eng., Hiroshima Univ., Higashihiroshima, 724, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1994),

67(2), 438-44
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In order to elucidate the relationship between the chem. structure and bitter taste of the C-terminal portion of .beta.-casein, H-Arg-Gly-Pro-X-Pro-Ile-Ile-Val-OH (I; X = Phe), analogs I (X = D-Phe, Lys, Gly, Glu, L-pyrenylalanine) were synthesized. Sensory analyses and CD spectra showed that the location of a hydrophobic amino acid with the L-configuration between the two proline residues should be important for this series of peptides to produce a strong bitterness.
IT **90600-53-6**, Bovine .beta.-casein (202-209)
RL: PRP (Properties)
(conformation of, by CD and bitter taste of)

L10 ANSWER 3 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1994:164859 CAPLUS
DOCUMENT NUMBER: 120:164859
TITLE: Syntheses of H-Arg-202-Gly-Pro-Phe-Pro-Ile-Ile-Val209-OH, corresponding to the C-terminal portion of .beta.-casein, and its analogs
AUTHOR(S): Nakatani, Masaru; Nakata, Takashi; Shinoda, Ichizo; Kouge, Katsushige; Okai, Hideo
CORPORATE SOURCE: Fac. Eng., Hiroshima Univ., Higashihiroshima, 724, Japan
SOURCE: Pept. Chem. 1992, Proc. Jpn. Symp., 2nd (1993), Meeting Date 1992, 424-6. Editor(s): Yanaihara, Noboru. ESCOM: Leiden, Neth.
CODEN: 59NTAC
DOCUMENT TYPE: Conference
LANGUAGE: English
AB A report from a symposium on he prepn. and conformation of the title bitter-tasting octapeptide and analogs.
IT **90600-53-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn., bitter taste, and conformation of)

L10 ANSWER 4 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1993:473097 CAPLUS
DOCUMENT NUMBER: 119:73097
TITLE: Convenient synthesis of flavor peptides
AUTHOR(S): Nakatani, Masaru; Okai, Hideo
CORPORATE SOURCE: Fac. Eng., Hiroshima Univ., Higashi-Hiroshima, 724, Japan
SOURCE: ACS Symposium Series (1993), 528(Food Flavor and Safety), 149-57
CODEN: ACSMC8; ISSN: 0097-6156
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A symposium report on the large-scale prepn. of flavor proteins and peptides by protein recombination methods and by enzymic synthesis using chem.-modified enzymes. The protein recombination method was applied to the synthesis of the C-terminal portion of .beta.-casein, and an org. solvent-stable modified chymotrypsin was used in the 1-step synthesis of inverted aspartame-type sweetener Ac-Phe-Lys-OH.
IT **90600-53-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, via enzymic couplings and modifications)

L10 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1991:3940 CAPLUS
DOCUMENT NUMBER: 114:3940
TITLE: Studies on flavored peptides. VIII. Mechanism for

the bitter tasting potency of peptides using O-aminoacyl sugars as model compounds
AUTHOR(S): Tamura, Masahiro; Miyoshi, Takafumi; Mori, Naoko; Kinomura, Keisuke; Kawaguchi, Michihiko; Ishibashi, Norio; Okai, Hideo
CORPORATE SOURCE: Fac. Eng., Hiroshima Univ., Higashi-Hiroshima, 724, Japan
SOURCE: Agricultural and Biological Chemistry (1990), 54(6), 1401-9
CODEN: ABCHA6; ISSN: 0002-1369
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In order to study the role of hydrophobicity in bitter peptides, several O-aminoacyl sugars, in which amino acids or peptides were attached to the 2- and 3-position of Me .alpha.-D-glucopyranoside, were synthesized and tasted. The bitterness increased as the hydrophobicity increased, implying that the bitterness receptor recognizes the hydrophobicity of bitter peptides. The bitterness receptor structure also is discussed.
IT **90600-53-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(bitterness of, hydrophobicity in relation to)

L10 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1986:532413 CAPLUS
DOCUMENT NUMBER: 105:132413
TITLE: Bitter taste of the carboxy-terminal tetradecapeptide of bovine .beta.-casein, -PRO196-VAL-LEU-GLY-PRO-VAL-ARG-GLY-PRO-PHE-PRO-ILE-ILE-VAL209
AUTHOR(S): Kato, Hironobu; Shinoda, Ichizo; Fushimi, Akira; Okai, Hideo
CORPORATE SOURCE: Fac. Eng., Hiroshima Univ., Shitami, 724, Japan
SOURCE: Peptide Chemistry (1986), Volume Date 1985, 23rd, 281-6
CODEN: PECHDP; ISSN: 0388-3698
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The bitter taste of the C-terminal portion of .beta.-casein, peptide 196-209 (I) [99909-33-8] and some of its fragments and analogs was examd. Threshold values were compared with that of caffeine, a std. bitter substance. The threshold value for I was 0.015 mM and for peptide 202-209 [**90600-53-6**] and peptide 200-209 [104160-90-9], the most bitter of the series, it was 0.004 mM. The 3 peptides had similar CD spectra, suggesting similarity in spacial structure. Comparison of the retro forms showed that the no. of hydrophobic amino acids was not the only factor in producing bitterness. Spatial structure and the presence of an N-terminal basic amino acid were also important parameters.
IT **90600-53-6**
RL: PRP (Properties)
(bitterness of, casein C-terminal peptides in relation to)

L10 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1986:66708 CAPLUS
DOCUMENT NUMBER: 104:66708
TITLE: Studies of bitter peptides from casein hydrolyzate. Part XI. Bitter taste of synthetic C-terminal tetradecapeptide of bovine .beta.-casein, H-Pro196-Val-Leu-Gly-Pro-Val-Arg-Gly-Pro-Phe-Pro-Ile-Ile-Val209-OH, and its related peptides
AUTHOR(S): Shinoda, Ichizo; Fushimi, Akira; Kato, Hironobu; Okai, Hideo; Fukui, Sakuzo
CORPORATE SOURCE: Fac. Eng., Hiroshima Univ., Higashihiroshima, 724, Japan

Searched by Barb O'Bryen, STIC 308-4291

SOURCE: Agricultural and Biological Chemistry (1985), 49(9), 2587-96
CODEN: ABCHA6; ISSN: 0002-1369
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The primary structure of bovine .beta.-casein contains the partial sequence of Pro196-Val-Leu-Gly-Pro-Val-Arg-Gly-Pro-Phe-Pro-Ile-Ile-Val209 in the C-terminal portion. The synthetic C-terminal octapeptide, Arg202-Val209, is extremely bitter with its threshold value 0.004 mM, 250 times as strong as that of caffeine [58-08-2]. To further investigate the bitter taste of the C-terminal portion of .beta.-casein, the C-terminal tetradecapeptide, Pro196-Val209, and some of its fragments were synthesized. A hydrophobic hexapeptide, Pro196-Val201, was twice as bitter as caffeine. The bitter taste of the decapeptide, Pro200-Val209, was the same as that of Arg202-Val209. Although the tetradecapeptide, Pro196-Val209, was composed of 2 bitter peptides, Pro196-Val201 and Arg202-Val209, its bitter taste was weaker than that of Arg202-Val209 and its threshold value was 0.015 mM. Probably the increase of bitterness in peptides through the introduction of hydrophobic amino acids depended on the no. of hydrophobic amino acids added. In addn., the synthetic retro analog of Arg202-Val209 (H-Val-Ile-Ile-Pro-Phe-Pro-Gly-Arg-OH) was not as bitter as Arg202-Val209. This indicated that the sequence of Arg202-Val209 is important for extreme bitterness.

IT **90600-53-6**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(bitterness of, mol. structure and .beta.-casein in relation to)

L10 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1984:423930 CAPLUS
DOCUMENT NUMBER: 101:23930
TITLE: Studies of bitter peptides from casein hydrolyzate. X. Synthesis and bitter taste of H-Arg-Gly-Pro-Phe-Pro-Ile-Ile-Val-OH corresponding to the C-terminal portion of .beta.-casein
AUTHOR(S): Kanehisa, Hidenori; Miyake, Ichizo; Okai, Hideo; Aoyagi, Haruhiko; Izumiya, Nobuo
CORPORATE SOURCE: Fac. Eng., Hiroshima Univ., Higashihiroshima, 724, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1984), 57(3), 819-22
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English

AB H-Arg-Gly-Pro-Phe-Pro-Ile-X-Val-OH [X = Ile (I) or null] were prepd. by conventional soln. methods. I and synthetic bitter peptide BPIa (H-Arg-Gly-Pro-Pro-Phe-Ile-Val-OH) do not match on thin-layer chromatog. The result indicates that BPIa does not correspond to the C-terminal portion of .beta.-casein as detd. by R. B. Dumas et al. (1972). The octapeptide posseses an extremely bitter taste.

IT **90600-53-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and bitter taster of)

=> fil hom
FILE 'HOME' ENTERED AT 15:56:52 ON 27 FEB 2003